Out of equilibrium statistical ensembles for mesoscopic rings coupled to reservoirs

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We derive non equilibrium statistical ensembles for a ballistic Aharonov-Bohm loop connected to several electrodes connected to reservoirs with different chemical potentials. A striking consequence of these non trivial ensembles is the emergence of quantum zero point fluctuations of the persistent current around the loop. Detailed predictions for the low frequency noise power are given.

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Persistent currents in isolated rings have been the subject of detailed theoretical [1, 2] and experimental [3, 4, 5, 6] investigations. They are indeed a probe of the many body energy level dependance in the external magnetic flux but they are also sensitive to the quantum state of the ring. Persistent currents in isolated mesoscopic networks have been discussed theoretically in the context of a semi-classical model in the diffusive limit [7], and in the context of the scattering approach for ballistic conductors [8]. Observation of persistent currents in an isolated set of connected mesoscopic diffusive rings has been reported in recent experiments [9].

The physics associated to persistent currents in a ring connected to external reservoirs has first been investigated in [10] where the connection between the spectrum of the isolated ring and its transport properties in a two terminal geometry has been established. The resulting h/e periodic oscillations of the conductance have been observed experimentally [11]. Connecting a circuit (which plays the role of the *system*) to external leads will also affect the persistent current because of the electron's tunnelling into the leads. For instance, connection to a single lead has been considered in [12] to model dissipation in the ring. Here, we investigate deeply non-equilibrium situations such as a two terminal experiment with a high bias voltage. In the non-equilibrium case, the reduced density matrix of the ring is a non trivial one, not reducible to any equilibrium density matrix. This effect is non perturbative since it survives even in the limit of vanishing coupling to the reservoirs.

In this letter, we illustrate this idea in the simple example of a mesoscopic ballistic non interacting ring coupled to several electrodes that are connected to external reservoirs of different chemical potentials. We first determine the ring's reduced density matrix and show that it can be used to recover transport properties in the spirit of [10]. Then, we show that a dramatic signature of the non equilibrium character of the ring's reduced density matrix is the presence of quantum zero point fluctuations of the persistent current around the ring. With progresses of low noise measurements and nano-fabrication techniques, these fluctuations may become observable in a near future. This effect is basically due to the increase of electron states that contribute to the noise. Let us mention that increases of shot noise based on the same general idea have also been discussed in the context of beam experiments [13] and of diffusive contacts with strong electron/electron interactions [14]. We end this letter by discussing how these non-equilibrium issues can be traced within the framework of Keldysh's formalism.

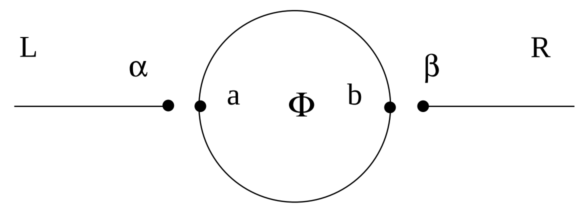

FIG. 1: Two terminal geometry for a mesoscopic Aharonov-Bohm ring threaded by a magnetic flux Φ.

Similarly to Ref. [8], we divide a connected system into two types of regions: a ballistic "intermediate" region that contains an Aharonov-Bohm loop and external electrodes connected to the Aharonov-Bohm loop (see Fig. 1). DC-transport can be controlled through a voltage difference V applied between the left and right external electrodes and the flux enclosed by the Aharonov-Bohm loop. Quantities of physical interest are the transport current flowing across the mesoscopic device and the persistent current flowing around the loop.

The external electrodes and the intermediate region can be described using a tight-binding Hamiltonian for free electrons. The coupling between the left/right electrodes and the intermediate island is described by the tunnel Hamiltonian :

$$\hat{\mathcal{W}} = t_{a,\alpha} c_a^+ c_\alpha + t_{\alpha,a} c_\alpha^+ c_a + t_{b,\beta} c_b^+ c_\beta + t_{\beta,b} c_\beta^+ c_b. \quad (1)$$

Since we are interested in out of equilibrium effects, we focus on the $eV \gg k_B T$ regime. In most cases, we shall set $T =$ 0 K. This model is valid provided that the tunnelling amplitudes from the electrodes to the small sys-

tem are much larger than the inelastic scattering rates inside the small system. In this case, tunnelling to the electrodes completely determine the non equilibrium state of the system and reservoirs. The most transparent picture of this stationary non equilibrium state can be obtained within the Laudauer formalism. The idea of the scattering approach is to find a basis of stationary one-particle states (the "in" states) from which the exact non equilibrium many body state of the global system (mesoscopic device and leads) can be constructed. The prescription is then to fill the "in" states coming from each lead up to its chemical potential.

Since we are interested in the persistent current, a quantity specific to the small system, the natural object to consider is the one particule reduced density matrix restricted to the mesoscopic device. To our knowledge, this object has seldom been considered within the context of mesoscopic physics whereas it has been discussed long ago in the context of black hole physics. In the discussion of Unruh and Hawking effects [15], the degrees of freedom behind the horizon are the counterparts of those attached to the leads in the present case. The ring's one particle reduced density operator can be obtained by eliminating the one particle wave functions in the leads from the exact stationary Schrődinger equation. This procedure yields an inhomogeneous Schrődinger equation on the small system, with an effective Hamiltonian containing boundary terms representing hopping back and forth to the reservoirs and a source term associated to the incident electronic flux. Solutions to this equation provides the decomposition of "in" states's wave functions in the mesoscopic system's Hilbert space.

This decomposition has a very simple form in the limit of very small coupling to the leads. It shows Lorentzian resonances when the energy of the "in" state coincides with the one particle eigenvalue ε_λ of the isolated mesoscopic system's Hamiltonian. Near resonance, the decomposition of the "in" state coming from the left electrode at energy ε is given by:

$$\psi_\lambda(\varepsilon, L) \simeq \frac{i\, t_{\alpha,a}\, \langle\lambda|a\rangle}{(\varepsilon-\varepsilon_\lambda)+\frac{i\hbar}{2}\Gamma_\lambda}. \tag{2}$$

Here $\Gamma_\lambda = \frac{l}{\hbar^2 v_R}(|t_{\alpha,a}\langle a|\lambda\rangle|^2+|t_{\beta,b}\langle b|\lambda\rangle|^2)$ denotes the total escape rate given by the Fermi golden rule for an electron in the small system stationary state $|\lambda\rangle$ expressed in terms Fermi velocity in the reservoirs v_R and the lattice spacing l. From the lead's point of view, these resonances appear in the transmission coefficient:

$$t(\varepsilon) \simeq \frac{i\, t_{\alpha,a} t_{\beta,b}\, \langle b|\lambda\rangle\langle\lambda|a\rangle}{(\varepsilon-\varepsilon_\lambda)+\frac{i\hbar}{2}\Gamma_\lambda}. \tag{3}$$

In the case where the level spacing in the mesoscopic system is large compared to the total escape rate Γ_λ of an electron from the state $|\lambda\rangle$ to the electrodes, the ring's reduced density matrix is diagonal within the basis of one particle energy levels of the ring (incoherent reduced density matrix). Populations $\overline{n}(\varepsilon_\lambda) = \langle c_\lambda^\dagger c_\lambda\rangle$ are given at zero temperature by:

$$\overline{n}(\varepsilon_\lambda) = \frac{1}{2} - \frac{\Gamma_L}{\pi\Gamma}\arctan\left(\frac{\varepsilon_\lambda-\mu_L}{\hbar\Gamma/2}\right) - \frac{\Gamma_R}{\pi\Gamma}\arctan\left(\frac{\varepsilon_\lambda-\mu_R}{\hbar\Gamma/2}\right) \tag{4}$$

where $\Gamma_{L,R}$ denote the escape rates in the left (resp. right) electrode given by the Fermi golden rule. In general, these escape rates do depend on the energy level λ. Note that $\overline{n}(\varepsilon_\lambda)$ is nothing but the average of contributions of all electrodes connected to the small system, the ponderation being provided by ratios of Fermi golden rule's escape rates. In the limit of very small tunnelling amplitudes, this distribution can still remain non trivial, being a step function determined by the ratios of tunnelling amplitudes. The values of these non equilibrium populations are easily understood in a classical way according to the sequential tunnelling picture. For instance, when $\mu_L > \mu_R$ and for energy levels $\mu_R < \varepsilon_\lambda < \mu_L$, the current $(1-\overline{n}(\varepsilon_\lambda))\Gamma_L$ from the left lead must be equal to the current $\overline{n}(\varepsilon_\lambda)\Gamma_R$ to the right lead leading to a non equilibrium population Γ_L/Γ consistent with eq. (4). We note that local non equilibrium occupation numbers have been discussed and observed experimentally in mesoscopic diffusive wires [16].

For a non interacting system, the persistent current is the average value of the derivative of the ring's Hamiltonian with respect to the magnetic flux. Using the mesoscopic system's reduced density matrix and under the hypothesis of negligible variation of escape rates for all the energy levels which are partially occupied, a simple expression can be given in terms of the persistent current $I(\phi,\mu_\alpha)$ of a ring at fixed chemical potentiel μ_α:

$$I_P(\phi) = \sum_\alpha \frac{\Gamma_\alpha}{\Gamma}\, I(\phi,\mu_\alpha) \tag{5}$$

The current $I(\phi,\mu_\alpha)$ can be computed directly in term of the single electron eigenenergies $\varepsilon_n(\phi)$ for the isolated ring as $\sum_n \frac{d\varepsilon_n(\phi)}{d\phi}\,\Theta(\mu_\alpha-\varepsilon_n(\phi))$ or equivalently using the scattering matrix of the ring [17]. Formula (5) directly shows the influence of non equilibrium populations given by eq. (4). Let us also notice that, in this non equilibrium situation, the persistent current cannot be derived using the derivative of the average energy with respect to the flux. As a function of the external magnetic flux, the persistent current still roughly has a sawtooth shape but with discontinuities when one particle energy levels cross the reservoir's chemical potentials.

At fixed reservoir's chemical potentials, the experimental signal is given by the Fourier transform with respect to the magnetic flux. Let us recall that for an isolated ballistic 1D ring, the n-th harmonic I_n is given in terms of the Fermi velocity v_F, the ring's perimeter L and the number of electrons in the ring N. Introducing

$I_\star = ev_F/L$:

$$I_n = I_\star \times \frac{i}{\pi n}\,(-1)^{nN} \tag{6}$$

In the non equilibrium situation described here, at zero temperature, the harmonics are given by :

$$I_n[(\mu_\alpha)] = I_\star \times \frac{i}{\pi n}\,\times\left(\sum_\alpha \frac{\Gamma_\alpha}{\Gamma}\,\cos\left(2\pi n\chi(\mu_\alpha)\right)\right) \tag{7}$$

where $\chi(\mu) = \sqrt{\frac{2mL^2\mu}{h^2}}$ corresponds to an effective flux associated with the chemical potential μ. In the particular case of a two terminal geometry, the nth harmonic is modulated by the bias voltage V. As expected on physical grounds, the modulation only appears in the asymmetric case. Assuming that $eV = \mu_L - \mu_R$ is small compared to $\sqrt{\mu} = (\sqrt{\mu_L} + \sqrt{\mu_R})/2$, we have for the V-dependant part of n-th Fourier harmonic:

$$\frac{I_n[\mu_L,\mu_R]}{I_n[\mu,\mu]} - 1 = \frac{\Gamma_L - \Gamma_R}{\Gamma}\,\tan\left(2\pi n\chi(\mu)\right)\,\sin\left(\frac{n\,eVL}{\hbar v_F\sqrt{2}}\right) \tag{8}$$

In principle, this could be experimentally observed under conditions similar to the ones necessary for the observation of the persistent current in a single ballistic ring. We assume the effective electron gas temperature to be smaller than $\hbar v_F/L$. Tunnelling amplitudes must be within the range $k_BT/\hbar \ll \Gamma_{L/R} \ll v_F/L$ and the voltage bias should satisfy $eV \gg \hbar v_F/L$. For 10 μm diameter ring, the level spacing is typically of 500 mK. A temperature within the mK range ensures that thermal effects do not suppress the persistent current. Voltages above 1 mV should be sufficient to create non equilibrium populations for many one particle energy levels. The total dc-conductance is given by $G = \frac{e^2}{h}\,\frac{2L}{v_F}\,\frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}$.

A more striking signature of the non equilibrium reduced density matrix can be found in the zero temperature noise of the persistent current. Since the "in" scattering states are stationary states of the total Hamiltonian, the two time correlation function of the persistent current can be exactly computed using our previous expressions for $\psi_\lambda(\varepsilon,\alpha)$. Its Fourier transform $S_{I_P}(\omega)$ turns out to have a complicated expression showing quantum structures above frequencies of order Γ. For the ring considered above, at a dc-resistance of the order of 10 to 1000 h/e^2, this frequency is still above 1 Mhz. Measurements of the persistent current as carried for instance in [9] are done at a much lower frequency. Therefore, experimentalists only access to the zero frequency limit of the noise. $S_{I_P}(0)$ turns out to be related to the ensemble fluctuations $C_P = \langle I_P^2\rangle - \langle I_P\rangle^2$ of the persistent current by $S_{I_P}(0) = 2C_P/\Gamma$. At low frequency, $S_{I_P}(\omega)$ shows a lorentzian behaviour:

$$S_{I_P}(\omega) \simeq \frac{2\Gamma}{\omega^2+\Gamma^2}\,C_P. \tag{9}$$

The characteristic function of the probability distribution of the persistent current is given by a superposition of partition noises ($j_n(\phi) = d\varepsilon_n(\phi)/d\phi$):

$$\widehat{P}(k) = \prod_n \left(1 + \overline{n}(\varepsilon_n(\phi))(e^{ikj_n(\phi)} - 1)\right) \tag{10}$$

Only the partially populated energy levels contribute to the non-zero cumulants and therefore these non-zero cumulants constitute a true signature of the non equilibrium state of the ring. On the contrary, the persistent current of an isolated ring has zero noise at zero temperature. This opens the possibility of an experimental test although measuring the persistent current noise can be quite an experimental challenge.

The total noise is a sum of contributions associated to the partially occupied one particle energy levels. For $eV \gg \hbar v_F/L$, a continuum spectrum approximation can be used. Since all energy levels between the smallest and the largest lead's chemical potential contribute to the noise, the variation of the Fermi velocity $v_F(\varepsilon)$ might be taken into account for explicit evaluations. The variance C_P of the persistent current is finally obtained as:

$$C_P = I_\star^2 \int \frac{v_F(\varepsilon)}{v_F}\,\overline{n}(\varepsilon)(1-\overline{n}(\varepsilon))\,\frac{d\varepsilon}{\hbar v_F/L} \tag{11}$$

In particular, for the two terminal geometry, and assuming constant escape rates and constant Fermi velocity over the relevant energy range, one gets:

$$C_P = I_\star^2\,\frac{|eV|}{hv_F/L}\,\frac{\Gamma_L\Gamma_R}{\Gamma^2} \tag{12}$$

which shows that the fluctuation of the persistent current becomes larger than its average value as soon as the voltage is larger than the energy level separation in the ring. The three terminal geometry has a richer structure. Denoting by $\mu_{1,2,3}$ the chemical potentials in decreasing order and $y_\alpha = \Gamma_\alpha/\Gamma$, we get:

$$C_P = \frac{eI_\star^2}{hv_F/L}\left(V_2y_2(y_1-y_3) + V_3y_3(1-y_3) - V_1y_1(1-y_1)\right) \tag{13}$$

Note that sensitivity with respect to the intermediate voltage is enhanced with the asymmetry in the couplings to the leads.

As expected, the noise is also a periodic function of the magnetic flux. Its Fourier transform with respect to the magnetic flux can easily be obtained using the free electron dispersion relation. Using $v_F^2(\varepsilon_n(\phi))/v_F^2 = \varepsilon_n(\phi)/\varepsilon_F$, the zero temperature noise can be related to the persistent current around a loop connected to a single lead. Ordering the chemical potentials in increasing order, we get:

$$\frac{\partial C_P}{\partial\phi} = \frac{I_\star^2}{\varepsilon_F}\sum_\alpha (I_P(\phi,\mu_\alpha) - I_P(\phi,\mu_{\alpha+1}))\,\overline{n}_{\alpha,\alpha+1}(1-\overline{n}_{\alpha,\alpha+1}) \tag{14}$$

where $\overline{n}_{\alpha,\alpha+1}$ denotes the non equilibrium population of all energy levels between chemical potentials μ_α and $\mu_{\alpha+1}$. In the end, the n-th harmonic of the zero temperature variance of the persistent current is given by:

$$C_P(n) = \frac{I_\star^2}{2\pi^2 n^2} \sum_{\beta\neq\alpha} y_\alpha y_\beta \,\mathrm{sign}(\alpha-\beta)\, \cos\left(2\pi n\chi(\mu_\alpha)\right) \tag{15}$$

Let us now connect the simple physical picture just developed to some important issues raised within the Keldysh approach. The Keldysh formalism is a natural framework for dealing with non equilibrium physics [18]. It provides a way to do systematic perturbation theory in the tunnelling amplitudes. The starting point of this perturbation theory is an "initial" density operator which is partly fixed by imposing the temperatures and chemical potentials of the external reservoirs. But this does not by itself determine the initial density operator for the mesoscopic ring.

In order to clarify this point, let us discuss the dc-current through system. The current flowing through the left contact can be expressed as [19]:

$$I_{\alpha,a} = \frac{e^2|t_{\alpha,a}|^2}{\hbar}\,(G^<_{aa}g^>_{\alpha\alpha} - G^>_{aa}g^<_{\alpha\alpha}). \tag{16}$$

where the $g_{\alpha\alpha}$s denote Keldysh's Green functions for the isolated left lead whereas the $G_{a,a}$s are for the system with the right lead connected. Using Dyson's equation, one gets: $G^<_{a,a} = (1+G^Rt)g^<(1+tG^A)$. Naively, equation (16)'s r.h.s. could depend on the system's initial density operator through Keldysh's Green functions for the isolated mesoscopic system. Such terms would introduce infrared divergences in Keldysh's perturbative expansion and of course be present in computations involving the persistent current around the ring. But the key point is that Dyson's equation for the retarded and advanced Green's function provide a way to cure this problem in the non interacting case since one can show that $1+G^Rt = G^R(g^R)^{-1}$ vanishes on the system's eigenenergies. Those terms can also be cured order by order in Keldysh's perturbative expansion by imposing that the system's "initial" Green's function $g^{>,<}$ are given by the non trivial one particle reduced density operator computed in this letter.

Similar issues have been recently discussed in the context of quantum dots. For example, in Ref. [20], the authors ask how to represent the effect of a large voltage bias between the two leads connected to a dot in the Kondo regime. This particular problem raises the important question of finding the correct starting point for Keldysh's perturbative expansion in the coupling to the reservoirs. In a recent work [21], O. Parcollet and C. Hooley have pointed out the importance of finding the right reduced density operator for the impurity spin even in the limit of a small coupling to the leads in order to obtain a well defined and correct perturbation expansion.

In conclusion, we have shown on a specific example that the physics of mesoscopic devices connected to external leads must be described using non equilibrium statistical ensembles even in the limit of vanishing coupling to the reservoirs. The example of a mesoscopic ring connected to two leads at different voltages could provide a direct experimental test of these ideas. We have shown that non zero cumulants of the persistent current are a signature of the non-equilibrium reduced density matrix of the mesoscopic ring. These ideas can be extended to more complicated circuits using the scattering approach on general graphs [22]. Another issue is to derive the non equilibrium state of an interacting system such as a Luttinger liquid coupled to leads.

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